

10/660,556

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NEWS 7 SEP 27 SWETSCAN will no longer be available on STN
NEWS 8 OCT 28 KOREAPAT now available on STN
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NEWS EXPRESS OCTOBER 29 CURRENT WINDOWS VERSION IS V7.01A, CURRENT
MACINTOSH VERSION IS V6.0c(ENG) AND V6.0Jc(JP),
AND CURRENT DISCOVER FILE IS DATED 11 AUGUST 2004
NEWS HOURS STN Operating Hours Plus Help Desk Availability
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* * * * * STN Columbus * * * * *

FILE 'HOME' ENTERED AT 08:10:54 ON 23 NOV 2004

=> file reg

COST IN U.S. DOLLARS

SINCE FILE

TOTAL

ENTRY

SESSION

FULL ESTIMATED COST

0.21

0.21

FILE 'REGISTRY' ENTERED AT 08:11:15 ON 23 NOV 2004

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STRUCTURE FILE UPDATES: 21 NOV 2004 HIGHEST RN 785750-23-4
DICTIONARY FILE UPDATES: 21 NOV 2004 HIGHEST RN 785750-23-4

TSCA INFORMATION NOW CURRENT THROUGH MAY 21, 2004

Please note that search-term pricing does apply when
conducting SmartSELECT searches.

Crossover limits have been increased. See HELP CROSSOVER for details.

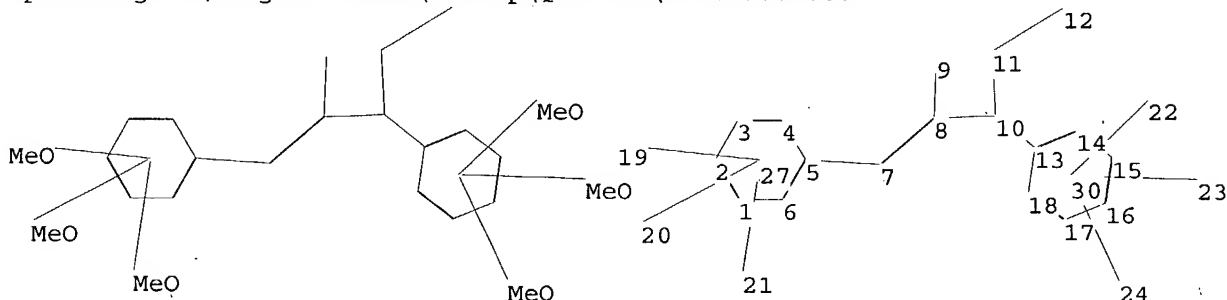
Experimental and calculated property data are now available. For more
information enter HELP PROP at an arrow prompt in the file or refer
to the file summary sheet on the web at:
<http://www.cas.org/ONLINE/DBSS/registryss.html>

=>Testing the current file.... screen

ENTER SCREEN EXPRESSION OR (END):end

=>

Uploading C:\Program Files\Stnexp\Queries\10660556c.str



chain nodes :

7 8 9 10 11 12 19 20 21 22 23 24

ring nodes :

1 2 3 4 5 6 13 14 15 16 17 18

chain bonds :

5-7 7-8 8-9 8-10 10-11 10-13 11-12

ring bonds :

1-2 1-6 2-3 3-4 4-5 5-6 13-14 13-18 14-15 15-16 16-17 17-18

exact bonds :

5-7 7-8 8-9 8-10 10-11 10-13 11-12

normalized bonds :

1-2 1-6 2-3 3-4 4-5 5-6 13-14 13-18 14-15 15-16 16-17 17-18

isolated ring systems :

containing 1 : 13 :

Match level :

1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:CLASS 8:CLASS 9:CLASS 10:CLASS
11:CLASS 12:CLASS 13:Atom 14:Atom 15:Atom 16:Atom 17:Atom 18:Atom 19:CLASS
20:CLASS 21:CLASS 22:CLASS 23:CLASS 24:CLASS 25:CLASS 26:CLASS 27:CLASS
28:CLASS 29:CLASS 30:CLASS

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L1 STRUCTURE UPLOADED

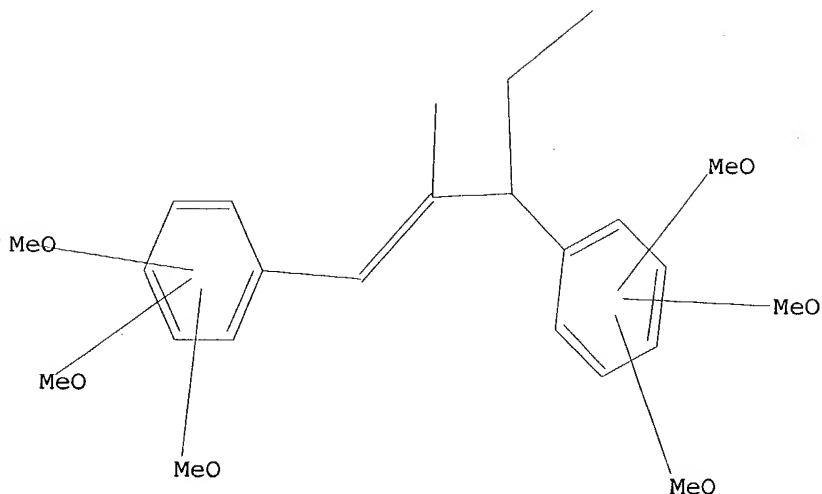
=> que L1

L2 QUE L1

=> d

L2 HAS NO ANSWERS

L1 STR



Structure attributes must be viewed using STN Express query preparation.

L2 QUE L1

=> s l2

SAMPLE SEARCH INITIATED 08:11:36 FILE 'REGISTRY'

SAMPLE SCREEN SEARCH COMPLETED - 140 TO ITERATE

100.0% PROCESSED 140 ITERATIONS
SEARCH TIME: 00.00.01

0 ANSWERS

FULL FILE PROJECTIONS: ONLINE **COMPLETE**
BATCH **COMPLETE**

PROJECTED ITERATIONS: 2091 TO 3509
PROJECTED ANSWERS: 0 TO 0

L3 0 SEA SSS SAM L1

=> s l2 ful

FULL SEARCH INITIATED 08:11:43 FILE 'REGISTRY'

FULL SCREEN SEARCH COMPLETED - 3331 TO ITERATE

100.0% PROCESSED 3331 ITERATIONS
SEARCH TIME: 00.00.01

2 ANSWERS

L4 2 SEA SSS FUL L1

=> d scan

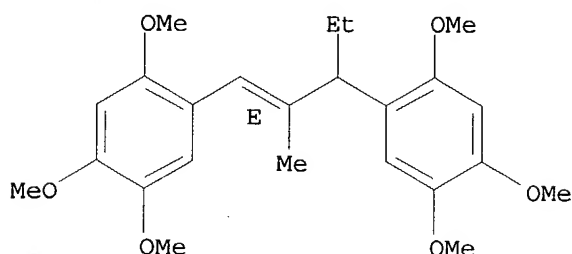
L4 2 ANSWERS REGISTRY COPYRIGHT 2004 ACS on STN

IN Benzene, 1,1'-[(1E)-3-ethyl-2-methyl-1-propene-1,3-diyl]bis[2,4,5-

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trimethoxy- (9CI)
MF C24 H32 O6

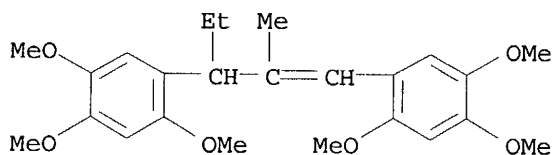
Double bond geometry as shown.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):1

L4 2 ANSWERS REGISTRY COPYRIGHT 2004 ACS on STN
IN Benzene, 1,1'-(3-ethyl-2-methyl-1-propene-1,3-diyl)bis[2,4,5-trimethoxy-
(9CI)
MF C24 H32 O6



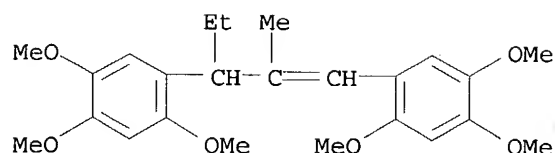
PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

ALL ANSWERS HAVE BEEN SCANNED

=> d 1-2

L4 ANSWER 1 OF 2 REGISTRY COPYRIGHT 2004 ACS on STN
RN 156246-57-0 REGISTRY
CN Benzene, 1,1'-(3-ethyl-2-methyl-1-propene-1,3-diyl)bis[2,4,5-trimethoxy-
(9CI) (CA INDEX NAME)
FS 3D CONCORD
MF C24 H32 O6
SR CA
LC STN Files: CA, CAPLUS, CASREACT
DT.CA Caplus document type: Journal; Patent
RL.P Roles from patents: PREP (Preparation); RACT (Reactant or reagent)
RL.NP Roles from non-patents: FORM (Formation, nonpreparative); PREP
(Preparation)

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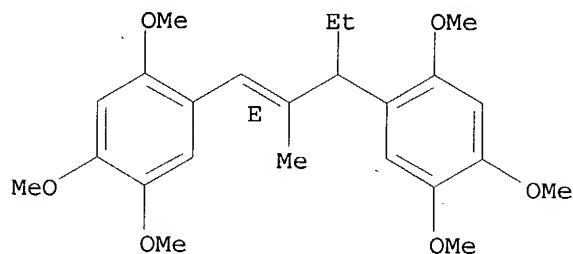


PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

2 REFERENCES IN FILE CA (1907 TO DATE)
2 REFERENCES IN FILE CAPLUS (1907 TO DATE)

L4 ANSWER 2 OF 2 REGISTRY COPYRIGHT 2004 ACS on STN
RN 80423-94-5 REGISTRY
CN Benzene, 1,1'-[(1E)-3-ethyl-2-methyl-1-propene-1,3-diyl]bis[2,4,5-trimethoxy- (9CI) (CA INDEX NAME)
OTHER CA INDEX NAMES:
CN Benzene, 1,1'-(3-ethyl-2-methyl-1-propene-1,3-diyl)bis[2,4,5-trimethoxy-, (E)-
OTHER NAMES:
CN Diasarone 1
CN NEOLASA-I
FS STEREOSEARCH
DR 130766-51-7, 82373-98-6
MF C24 H32 O6
LC STN Files: BEILSTEIN*, CA, CAPLUS, CASREACT, NAPRALERT, USPATFULL
(*File contains numerically searchable property data)
DT.CA Caplus document type: Journal; Patent
RL.P Roles from patents: PREP (Preparation); RACT (Reactant or reagent)
RL.NP Roles from non-patents: FORM (Formation, nonpreparative); PREP (Preparation); PRP (Properties); RACT (Reactant or reagent)

Double bond geometry as shown.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

5 REFERENCES IN FILE CA (1907 TO DATE)
5 REFERENCES IN FILE CAPLUS (1907 TO DATE)

=> file ca caplus
COST IN U.S. DOLLARS

SINCE FILE	TOTAL
ENTRY	SESSION
159.80	160.01

FULL ESTIMATED COST

FILE 'CA' ENTERED AT 08:13:08 ON 23 NOV 2004
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=> s 14

L5 14 L4

=> dup rem 15

PROCESSING COMPLETED FOR L5

L6 7 DUP REM L5 (7 DUPLICATES REMOVED)

=> d 1-7 bib ab

L6 ANSWER 1 OF 7 CA COPYRIGHT 2004 ACS on STN DUPLICATE 1

AN 139:292100 CA

TI Formation of neolignan by DDQ mediated dimerization of dihydroasarone

IN Sinha, Arun Kumar; Joshi, Bhupendra Prasad; Acharya, Ruchi

PA Council of Scientific and Industrial Research, India

SO PCT Int. Appl., 37 pp.

CODEN: PIXXD2

DT Patent

LA English

FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	WO 2003080551	A1	20031002	WO 2002-IN73	20020327
	W:	AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, OM, PH, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZM, ZW			
	RW:	GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG			

PRAI WO 2002-IN73

20020327

OS CASREACT 139:292100

AB The present invention relates to a novel neolignan 3-ethyl-2-methyl-3-(2'',4'',5''-trimethoxyphenyl)-1-(2',4',5'-trimethoxyphenyl)-1-propene and a process for the preparation of high purity, high yield neolignan, α -asarone, and 2,4,5-trimethoxyphenylpropionone from β -asarone or β -asarone rich Acorus calamus oil containing α - and γ -asarone by hydrogenating and dimerizing by treatment with DDQ in presence of an organic acid.

RE.CNT 4 THERE ARE 4 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L6 ANSWER 2 OF 7 CA COPYRIGHT 2004 ACS on STN DUPLICATE 2

AN 139:292099 CA

TI DDQ-mediated one step dimerization of β -asarone or β -asarone rich Acorus calamus oil in the formation of novel neolignan

IN Sinha, Arun Kumar; Joshi, Bhupendra Prasad; Acharya, Ruchi

PA Council of Scientific & Industrial Research, India

SO U.S. Pat. Appl. Publ., 20 pp.

CODEN: USXXCO

DT Patent

LA English

FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	US 2003187306	A1	20031002	US 2002-108269	20020328
	US 2004049085	A1	20040311	US 2003-660556	20030912
PRAI	US 2002-108269	B3	20020328		
OS	CASREACT 139:292099				
AB	The present invention relates to a novel neolignan, 3-ethyl-2-methyl-3-(2'',4'',5''-trimethoxyphenyl)-1-(2',4',5'-trimethoxyphenyl)-1-(2',4',5'-trimethoxy)phenyl-1-propene [NEOLASA-I (I)], and a process for the preparation of high purity, higher yield neolignan, α -asarone, 2,4,5-trimethoxy-phenylpropionone from β -asarone (II) or β -asarone rich Acorus calamus oil containing α - and γ -asarone by hydrogenating and dimerizing by treatment with DDQ in presence of an organic acid.				
L6	ANSWER 3 OF 7	CA	COPYRIGHT 2004 ACS on STN	DUPLICATE 3	
AN	121:82863	CA			
TI	Chemical structure of 1,3-bis(2,4,5-trimethoxy)phenyl-2-methyl-pentene-1				
AU	Liu, Buming; Ye, Chao; Jiang, Weiheng				
CS	Guangxi Inst. Traditional Med. Pharm., Nanning, 530022, Peop. Rep. China				
SO	Fenxi Huaxue (1994), 22(4), 355-8				
	CODEN: FHHHDT; ISSN: 0253-3820				
DT	Journal				
LA	Chinese				
AB	A new compound of lignans separated from the mother liquor of recrystn. in industrial synthesis of α -asaricin was reported. The structure of the compound was determined by UV, IR, ¹ H-NMR, ¹³ C-NMR and MS, and revealed to be 1,3-bis(2,4,5-trimethoxy)phenyl-2-methyl-1-pentene (I). The compound was synthesized by photochem. reaction using the above mentioned mother liquor. A possible reaction mechanism was also discussed.				
L6	ANSWER 4 OF 7	CA	COPYRIGHT 2004 ACS on STN	DUPLICATE 4	
AN	115:278048	CA			
TI	Light-induced transformation of asarone				
AU	Lander, V.; Schreier, P.				
CS	Univ. Wuerzburg, Wuerzburg, D-8700, Germany				
SO	Flavour and Fragrance Journal (1991), 6(1), 21-8				
	CODEN: FFJOED; ISSN: 0882-5734				
DT	Journal				
LA	English				
AB	The stability of α -(I) and β -asarone (II) in ethanolic solns. was studied under daylight conditions over a period of 6 mo. After rapid initial light-induced isomerization of I to II, a number of oxidation products, i.e. 2,4,5-trimethoxybenzaldehyde, 1-(2,4,5-trimethoxyphenyl)propan-2-one, and 2,4,5-trimethoxypropiophenone and addition products, i.e. 1-ethoxy-1-(2,4,5-trimethoxyphenyl)propane, (1R,2R; 1S,2S)-1-ethoxy-1-(2,4,5-trimethoxyphenyl)propan-2-ol, (1R,2S; 1S,2R)-1-ethoxy-1-(2,4,5-trimethoxyphenyl)propan-2-ol, (1R,2R; 1S,2S)-1-(2,4,5-trimethoxyphenyl)propan-1,2-diol, and (1R,2S; 1S,2R)-1-(2,4,5-trimethoxyphenyl)propan-1,2-diol, as well as the dimers 1-(2',4',5'-trimethoxyphenyl)-2-methyl-3-(2,4,5-trimethoxyphenyl)-1E-pentene (III) and 1-(2',4',5'-trimethoxyphenyl)-2-methyl-3-ethyl-1 α ,2 β ,3 α (II)-4,6,7-trimethoxyindane (IV) were detected after extractive sample preparation. In addition, 3 dimers, 1-(2',4',5'-trimethoxyphenyl)-2-methyl-3(2,4,5-trimethoxyphenyl)-penta-1E,4-diene, 1-(2',4',5'-trimethoxyphenyl)-2-(2,4,5-trimethoxyphenyl)-3,4-dimethylcyclobutane, and 1-(2',4',5'-trimethoxyphenyl)-2-methyl-3-(2,4,5-trimethoxyphenyl)prop-1-en-3-one were tentatively identified. Identification was carried out by capillary gas chromatog. (HRGC) and online HRGC techniques, i.e. HRGC mass spectrometry and HRGC-Fourier transform IR spectroscopy as well as ¹ H-NMR spectroscopy.				

L6 ANSWER 5 OF 7 CA COPYRIGHT 2004 ACS on STN DUPLICATE 5
 AN 113:241942 CA
 TI Structure of (E)-2-methyl-1,3-bis(2,4,5-trimethoxyphenyl)-1-pentene and
 1-(2,4,5-trimethoxyphenyl)-2-methyl-3-ethyl-4,6,7-trimethoxyindan
 C24H32O6: two asarone dimers
 AU Lemini, C.; Mandoki, J. J.; Cruz-Almanza, R.; Toscano, R. A.
 CS Fac. Med., UNAM, Coyoacan, 04510, Mex.
 SO Acta Crystallographica, Section C: Crystal Structure Communications
 (1990), C46(8), 1542-5
 CODEN: ACSCEE; ISSN: 0108-2701
 DT Journal
 LA English
 AB (E)-2-Methyl-1,3-bis(2,4,5-trimethoxyphenyl)-1-pentene (I) is monoclinic,
 space group P21/n, with a 7.082(3), b 11.954(7), c 27.136(17) Å, and
 β 94.14(4)°; d.(calculated) = 1.21 for Z = 4. Final R = 0.056 and
 Rw = 0.063 for 2901 reflections. 1-(2,4,5-Trimethoxyphenyl)-2-methyl-3-
 ethyl-4,6,7-trimethoxyindan (II) is monoclinic space group P21/a with a
 17.281(5), b 7.701(1), c 18.057(6) Å, and β 108.23(2)°;
 d.(calculated) = 1.21 for Z = 4. Final R = 0.045 and Rw = 0.061 for 2601
 reflections. Atomic coordinates are given. The x-ray structures confirm the
 structures previously assigned on the basis of chemical and NMR spectral
 evidence. I is non-planar. In II the 5-membered ring adopts an envelope
 conformation and the substituents at C(1) and C(3) are antiperiplanar to
 the Me group at C(2). In both isomers the orientation of the
 trimethoxyphenyl substituent is determined by C-H...O intramol. interactions.
 The packing in the crystal is entirely due to van der Waals forces.

L6 ANSWER 6 OF 7 CA COPYRIGHT 2004 ACS on STN DUPLICATE 6
 AN 97:38740 CA
 TI The active substances of Asarum europaeum L. XV. Structure of the
 diasarones
 AU Bohlmann, Ferdinand; Gracza, Lajos
 CS Inst. Org. Chem., Tech. Univ. Berlin, Berlin, D 1000, Fed. Rep. Ger.
 SO Archiv der Pharmazie (Weinheim, Germany) (1982), 315(5), 474-6
 CODEN: ARPMAS; ISSN: 0365-6233
 DT Journal
 LA German
 AB Diasarone, prepared by the method of T. Szeki (1906), consists of 2
 substances, diasarone-1 (I) and diasarone-2 (II).

RS1.A7

L6 ANSWER 7 OF 7 CA COPYRIGHT 2004 ACS on STN DUPLICATE 7
 AN 96:34762 CA
 TI Synthesis of a novel asarone dimer
 AU Lemini, C.; Cruz, R.; Sanchez, I. H.
 CS Fac. Med., Univ. Nac. Auton. Mexico, Mexico City, Mex.
 SO Organic Preparations and Procedures International (1981), 13(5), 374-8
 CODEN: OPPIAK; ISSN: 0030-4948
 DT Journal
 LA English
 AB Title compds. I and II were prepared as anticholesteremics (no data). Thus,
 asarone was treated at room temperature with PBr3 for 3 h to give 87% E-I.
 Treating I with PBr3 for 24 h gave 78% II. I was converted to II by acid
 catalysis.

=> log y

COST IN U.S. DOLLARS

SINCE FILE

TOTAL

ENTRY

SESSION

FULL ESTIMATED COST

20.80

180.81

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)

SINCE FILE

TOTAL

10/660,556

CA SUBSCRIBER PRICE

ENTRY
-4.62

SESSION
-4.62

STN INTERNATIONAL LOGOFF AT 08:18:04 ON 23 NOV 2004